AD-A273 866

③

NAVAL POSTGRADUATE SCHOOL
Monterey, California

REPEATED KNOTS IN LEAST SQUARES

MULTIQUADRIC FUNCTIONS

by
Richard Franke
Hans Hagen
Gregory M. Nielson

93-30553

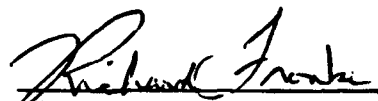## NAVAL POSTGRADUATE SCHOOL
MONTEREY, CA 93943
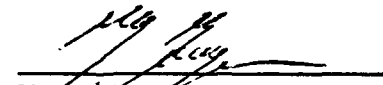
Rear Admiral T.A. Mercer
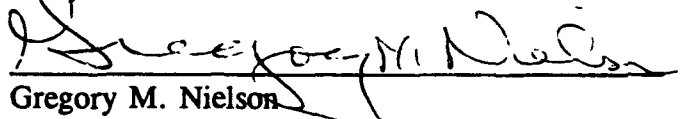Superintendent

Harrison Shull
Provost

This report was prepared in conjunction with research conducted for the Naval Postgraduate School and funded by the Naval Postgraduate School and the Office of Naval Research.

Reproduction of all or part of this report is authorized.
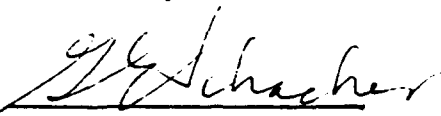
This report was prepared by:

Richard Franke
Professor of Mathematics

Hans Hagen
Professor of Mathematics

Gregory M. Nielson
Professor of Mathematics

Accesion For		
NTIS CRA&I		☑
DTIC TAB		☑
Unannounced		☐
Justification		
By		
Distribution /		
Availability Codes		
Dist	Avail and / or Special	
A-1		

Reviewed by:

GORDON SCHACHER
Dean of Faculty

Released by:

PAUL J. MARTO
Dean of Research

REPORT DOCUMENTATION PAGE		*Form Approved* OMB No 0704-0188

1a REPORT SECURITY CLASSIFICATION Unclassified	1b RESTRICTIVE MARKINGS

2a SECURITY CLASSIFICATION AUTHORITY	3 DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited
2b DECLASSIFICATION/DOWNGRADING SCHEDULE	

4 PERFORMING ORGANIZATION REPORT NUMBER(S) NPS-MA-94-004	5 MONITORING ORGANIZATION REPORT NUMBER(S) NPS-MA-94-004

6a NAME OF PERFORMING ORGANIZATION Naval Postgraduate School	6b OFFICE SYMBOL *(If applicable)* MA	7a NAME OF MONITORING ORGANIZATION Naval Postgraduate School
6c. ADDRESS (City, State, and ZIP Code) Monterey, CA 93943		7b ADDRESS (City, State, and ZIP Code) Monterey, CA 93943

8a NAME OF FUNDING/SPONSORING ORGANIZATION Naval Postgraduate School	8b OFFICE SYMBOL *(If applicable)* MA	9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER OM,N

8c. ADDRESS (City, State, and ZIP Code) Monterey, CA 93943	10 SOURCE OF FUNDING NUMBERS			
	PROGRAM ELEMENT NO	PROJECT NO	TASK NO	WORK UNIT ACCESSION NO

11 TITLE (Include Security Classification)
Repeated Knots in Least Squares Multiquadric Functions

12 PERSONAL AUTHOR(S)
Richard Franke, Hans Hagen, Gregory M. Nielson

13a TYPE OF REPORT Technical	13b TIME COVERED FROM 8-93 TO 10-93	14 DATE OF REPORT (Year, Month, Day) 14 Oct 93	15 PAGE COUNT 11

16 SUPPLEMENTARY NOTATION

17	COSATI CODES		18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number) Least squares multiquadric functions
FIELD	GROUP	SUB-GROUP	

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

A previous paper by the authors [FH93] noted that there was a strong tendency to obtain near-repeated knots in their algorithm for least squares approximation of scattered data by multiquadric functions. In this paper we observe that this leads naturally to the inclusion of derivatives of the multiquadric basis function in the approximation, and give an algorithm for accomplishing this. A comparison of the results obtained with this algorithm and the previous one is made. While the multiple knot algorithm usually has the advantage in terms of accuracy and computational stability, there are datasets for which this is reversed.

20 DISTRIBUTION/AVAILABILITY OF ABSTRACT ☐ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS	21 ABSTRACT SECURITY CLASSIFICATION Unclassified
22a NAME OF RESPONSIBLE INDIVIDUAL Richard Franke	22b TELEPHONE (Include Area Code) 408-656-2206	22c OFFICE SYMBOL MA/Fe

DD Form 1473, JUN 86   *Previous editions are obsolete*   SECURITY CLASSIFICATION OF THIS PAGE

REPEATED KNOTS IN LEAST SQUARES MULTIQUADRIC FUNCTIONS

Richard Franke*
Hans Hagen[†]
Gregory M. Nielson[‡]

October, 1993

Abstract

A previous paper by the authors [FH93] noted that there was a strong tendency to obtain near-repeated knots in their algorithm for least squares approximation of scattered data by multiquadric functions. In this paper we observe that this leads naturally to the inclusion of derivatives of the multiquadric basis function in the approximation, and give an algorithm for accomplishing this. A comparison of the results obtained with this algorithm and the previous one is made. While the multiple knot algorithm usually has the advantage in terms of accuracy and computational stability, there are datasets for which this is reversed.

*   Department of Mathematics, Naval Postgraduate School, Monterey, CA 93943

[†] FB Informatik, Universität Kaiserslautern, 67653 Kaiserslautern, Germany

[‡] Department of Computer Science, Arizona State University, Tempe, AZ 85287

1 Introduction

This paper continues an investigation into the use of multiquadric functions to approximate scattered data. An initial report on our efforts appears in [FH93], where we reported that a phenomenon that seemed particularly interesting was the tendency of the optimization process to result in near-repeated knots. The implication is that the method was attempting to build a directional derivative of the basis function into the approximation. This paper documents our experiences with an algorithm that detects the occurrence of near-repeated knots, and when they occur, replaces basis functions corresponding to near-repeated knots with a single multiquadric basis function plus appropriate derivatives of the multiquadric basis function, at the pertinent knot.

While it is useful to have the previous paper at hand, for completeness we will briefly review the background necessary to make this report somewhat self-contained. We restrict our discussion to functions of two independent variables, the methods are easily extendible to arbitrary dimensions, and we expect that many of the conclusions will carry over.

The scattered data approximation problem is easily described and occurs frequently in many branches of science. The problem occurs in any discipline where measurements are taken at irregularly spaced values of two or more independent variables, and is especially prevalent in environmental sciences. We will suppose that triples of data,(x_j, y_j, z_j), $j = 1, \cdots, N$ are given, assumed to be measurements (perhaps with error) of an underlying function $z = f(x, y)$. The function f is to be approximated by a function $F(x, y)$ from the given data. A recent survey of such methods is given in [FN91].

Multiquadric functions were introduced for interpolation of scattered data by Hardy [HA71]; also see [HA90] for a historical survey and many references. The method is one of a class of methods known now as "radial basis function methods" that includes other attractive schemes such as thin plate splines [HD72, DU76, and others]. The basic idea of such methods is quite simple, and we describe it in some generality; for purposes of being definite it is pertinent to note that for the multiquadric method the radial function is $h(d) = \sqrt{(d^2 + r^2)}$. In general, suppose a function of one variable, $h(d)$, where d denotes distance, is given.

For interpolation (that is, exact matching of the given data), a basis function, $B_j(x, y) = h(d_j)$ is associated with each data point. Here $d_j = \sqrt{((x - x_j)^2 + (y - y_j)^2)}$, the distance from (x, y) to (x_j, y_j). Thus each basis function is a translate of the radial function, h. The approximation is a linear combination of the basis functions, along with some polynomial terms that may be necessary in some cases, or may be used to assure that the approximation method has polynomial precision. Thus,

$$F(x, y) = \sum_{j=1}^{N} a_j B_j(x, y) + \sum_{j=1}^{M} b_j q_j(x, y) \qquad (1)$$

where $\{q_j\}$ is a set of M polynomials forming a basis for polynomials of degree $< m$. The coefficients a_j and b_j are determined by the linear system of equations prescribing interpolation

of the data, and exactness for polynomials of degree $< m$:

$$\sum_{j=1}^{N} a_j B_j(x_i, y_i) + \sum_{j=1}^{M} b_j q_j(x_i, y_i) = z_i, \ i = 1, \cdots, N$$

$$\sum_{j=1}^{N} a_j q_i(x_j, y_j) = 0, \ i = 1, \cdots, M. \tag{2}$$

For multiquadric basis functions, this system of equations is known to have a unique solution for distinct (x_j, y_j) data (see, for example, [MI86]); while m may be taken as zero (no polynomial terms), Micchelli's results show the multiquadric basis function is positive definite of order one, and thus a constant term should be included. We have done so in all our work. If higher degree polynomial precision is desired, inclusion of those terms imposes no particular burden.

While interpolation theory is important and indicates something about the suitability of the class of functions for approximation purposes, our emphasis here is on least squares approximation. This implies using fewer basis functions than there are data points. In analogy with univariate cubic splines, it is convenient to refer to the points at which the radial basis functions are centered as "knots", as was done in [MF92], and we do so here. If a set of knot points, $(u_k, v_k), k = 1, \cdots, K$, with $K < N$ have been specified, then the problem of fitting a multiquadric function by least squares is similar to that of solving the system of equations corresponding to those above in the least squares sense. We give the details. Now, let $B_k(x, y)$ denote the radial basis function associated with the point $(u_k, v_k), B_k(x, y) = \sqrt{((x - u_k)^2 + (y - v_k)^2 + r^2)}$. The system of equations, specialized for our case, is now of the form

$$\sum_{k=1}^{K} a_k B_k(x_i, y_i) + c = z_i, \ i = 1, \cdots, N$$

$$\sum_{k=1}^{K} a_k = 0. \tag{3}$$

There is a question of how to treat the last equation, which guarantees precision for constants. In [MF92] the corresponding constraint equations were imposed exactly, rather than approximately, because of physical considerations. While there is not the corresponding physical situation here, we have also imposed the last equation as a constraint. This constraint can be used to reduce the size of the system by solving for a_K in terms of the other a_k and substituting into the first set of equations.

If the knot points are a subset of the data points, then the system of equations (by virtue of containing, as a subset, interpolation equations) has full rank, and thus guarantees a unique solution of the least squares problem. When the knot locations may differ from the data points, the problem of whether the coefficient matrix is of full rank or not is unknown to us, although we feel certain that the matrix is of full rank when the knot points are distinct, and have encountered no situations that indicate otherwise.

The impetus behind our original investigation was to obtain surface approximations that would be efficient in subsequent applications. That is, we consider it to be acceptable to

expend considerable computational resources to obtain the approximation in a preprocessing step. Once obtained, the approximation can be evaluated efficiently, so it would be feasible to use it numerous times in an application program.

In the previous paper [FH93] we found that there was a tendency of the algorithm to converge on solutions where the knot points were often close to each other, or near-repeated. This occurred both in clusters of two and three knots. At that time, no attempt was made to made to investigate this behavior further. The outstanding result of that reference was the finding that allowing the knots (and r value) to be determined as part of the minimization process yielded approximations that were much more efficient than those obtained either by determining the knots a priori or adaptively (we outlined a greedy algorithm for sequentially determining knot locations that worked well). While we found that using variable r values also yielded good improvement, we do not pursue that idea here.

Because the greedy algorithm we developed previously was generally used as the starting point for the work reported here, we give a brief outline of it.

a) Obtain the least squares fit by a constant function, the average of the data values. The two data points having maximum positive and maximum negative error are taken to be the first two knots, (u_1, v_1) and (u_2, v_2). The knot counter K is set to 2.

b) The least squares multiquadric fit with K knots is obtained, and the residuals are computed.

c) The maximum absolute value of the residuals is found and the location of this residual, subject to the minimum knot separation value, is taken to be the next knot location (u_K, v_K). At this point the algorithm proceeds to step b unless the maximum number of knot locations to be computed has been reached.

As previously, we have used a QRP' decomposition of the coefficient matrix to solve the least squares problem for given knots and r value. This provides a stable and efficient means for solution of the problem with an indication if a matrix of less than full rank is encountered.

In order to test the algorithms we have used a number of data sets. Several of these are based on previously published and widely available (x, y) data sets and parent functions. We have also used a few less readily available data sets that we are willing to share with anyone interested in obtaining them. Table 1 gives a summary of most of the data sets.

As mentioned in the opening paragraph, the primary purpose of this paper is to discuss some further results we have obtained in allowing the coalescence of knots. A discussion of the algorithm we used is given in Section 2. Results of calculations obtained using several data sets and comparison with the previous method where only simple (but possibly near-repeated) knots are allowed, is given in Section 3. Section 4 summarizes our experiences.

n.m This refers to point set n and function m from [FR82], for $n =1$, 2, and 3, and $m = 1, \cdots, 6$. $n = 1$ is 25 points, $n = 2$ is 33 points, $n = 3$ is 100 points. $n = 4$ refers to the 200 point data set used in [MF92]. m=1 is the humps and dip function, $m = 2$ is the cliff, $m = 3$ is the saddle, $m = 4$ is the gentle hill, $m = 5$ is the steep hill, and $m = 6$ is the sphere. In addition, $m = 7$ refers to the curved valley function from [NI78].

GT This refers to the thinned glacier data consisting of 678 points, with certain contour lines removed, from [MF92].

GL This refers to the thinned glacier data consisting of 873 points.

HF This is the data set from [MF92] generated to have point density approximately proportional to curvature, consisting of 500 points.

Table 1: Data Sets Used Extensively in Tests

2 Derivatives of Multiquadric Basis Functions and Multiple Knots

Once again we have used Matlab [1] and LEASTSQ (a Levinburg-Marquardt method) to solve the nonlinear minimization problem

$$\min \sum_{i=1}^{N}[z_i - \sum_{k=1}^{K} a_k B_k(x_i, y_i) - c]^2 \tag{4}$$

where the minimization is taken over all (u_k, v_k), r, the a_k, and c (with the last equation of (3) imposed as a constraint) as an equivalent two step minimization. Thus, for each given knot configuration and r value, the least squares solution of (3) is computed as a step toward (4). This results in the solution of a simpler, but equivalent problem since $2K$ parameters are eliminated from (4) by imposing the condition that the values of the a_j and c be always taken as obtained from the least squares solution of (3). Hence, our final process is more properly written as

$$\min \min \sum_{i=1}^{N}[z_i - \sum_{k=1}^{N} a_k B_k(x_i, y_i) - c]^2 \tag{5}$$

where the inner minimization is over the a_j and c (least squares solution of (3)), and the outer minimization is over the knot locations and the value of the parameter r. The global minimum of each of the two problems are clearly the same. Eq. (5) is the more restrictive, but any minimum of (4) is a local minimum of (5), else a better solution is attainable for (4).

[1] MathWorks, 24 Prime Park Way, Natick. MA 01760

This does not imply that the iterative methods employed to solve (5) would work equally well, nor find the same local minima, when applied to (4).

When two knots approach each other, the system (3) becomes ill- conditioned, and the coefficients for the two knots tend to become large and of opposite sign. This reminds one of derivatives, in this case a directional derivative. Because the two coefficients are not of the same magnitude, the appropriate replacement basis functions seem to be one of the basis functions, and a directional derivative of the basis function. In practice, the directional derivative is represented as a linear combination of the partial derivatives with respect to x and to y. To prove this is the proper change requires showing that the coefficients grow at no greater a rate than the reciprocal of the distance between the knots. The work of Narcowich and Ward [NW91] shows that the norm of the inverse of the multiquadric interpolation matrix grows no more rapidly than linear with the reciprocal of the minimum distance between data points. It seems likely a similar result holds for the norm of the pseudoinverse of the system matrix for (3). We have verified this computationally for some cases.

The contribution of the two terms corresponding to the coalescent knots (say the jth and the kth) are of the form $a_j B_j(x,y) + a_k B_k(x,y)$. The six parameters, a_j, a_k, u_j, v_j, u_k, and v_k, in those terms are replaced by the five parameters in the terms $a_j B_j(x,y) + b_j(B_j(x,y))_x + c_j(B_j(x,y))_y$. In the previous expression the subscripts x and y refer to partial differentiation. We will refer to such a knot as a double knot.

Now, as it turns out, the coalescence of two knots, while the most prevalent, was by no means the only situation we encountered. The coalescence of three knots (or, once two knots have coalesced, the approach of a third knot to the location of a double knot) then results in the occurrence of a second derivative, a directional derivative of a directional derivative (the directions not necessarily being the same). In practice the replacement of the basis functions for the ith, jth, and kth knots is by the linear combination $a_j B_j + b_j(B_j)_x + c_j(B_j)_y + d_j(B_j)_{xx} + e_j(B_j)_{xy} + f_j(B_j)_{yy}$. While we have instances of near-coalescence of four knots, our present code does not attempt to handle such cases properly.

The algorithm is required to change basis functions when it appears that knots are coalescing. We have used a simple idea that seems to be effective. We iterate the solution of (5) in stages having increasingly stringent convergence tolerances. As each tolerance level is met, a check for near-repeated knots is made, "near" being a changing tolerance consistent with the tolerance for the optimization. When pairs of knots are found within the tolerance, the new basis is generated, and the optimization process continued. When no new repeated knots are obtained, the tolerance is decreased by a factor of two. We have observed that the inclusion of the derivative terms, vice the basis functions at near- repeated knots, generally yields essentially the same approximation, as it should, for both double and triple knots. The sequence of tolerance levels we used is: 0.02, 0.01, 0.005 for problems posed on the $[0,1]^2$ square.

3   Approximations with Repeated Knots

The results of our investigation concern the ability of the algorithm to obtain good approximations in comparison with the algorithm permitting only simple (but perhaps near-

repeated) knots, the degree of dependence on the initial guess for three different datasets (two in some detail), and a comparison of condition numbers of the coefficient matrices for the simple and multiple knot problems.

dset	r_s	r_m	rms_s	rms_m	$grms_s$	$grms_m$	$knots_s$	$knots_m$
3.1	0.0976	0.1588	0.0081	0.0059	0.0115	0.0107	2nd,1nt	1d,1t,1nt
3.2	7e-6	0.0002	0.0074	0.0073	0.0186	0.2477	3nd,1nt	3d,1t,1nq
3.3	0.3116	0.2502	0.0014	0.0008	0.0016	0.0011	1nt	1t
3.4	0.2885	0.3118	0.0005	0.0005	0.0006	0.0005	2nd	3d
3.5	0.3720	0.3886	0.0008	0.0007	0.0010	0.0010	3nd	2d
3.6	2.3280	2.3044	0.0005	0.0005	0.0007	0.0007		
3.7	0.0990	0.3304	0.0403	0.0279	0.0733	0.0324	4nd	4d
4.1	0.0958	0.1588	0.0070	0.0017	0.0071	0.0024	1nt	1t
4.2	2e-5	2e-5	0.0035	0.0035	0.0083	0.0082	4nd	3d,1nd
4.3	0.2577	0.2513	0.0002	0.0002	0.0002	0.0002	4nd	1d,1nd
4.4	0.4163	0.4625	7e-6	6e-6	7e-6	6e-6	1nd	3d
4.5	0.3234	0.3151	0.0002	0.0003	0.0002	0.0003	4nd	2nd
4.6	0.5668	0.5680	5e-5	4e-5	5e-5	4e-5	5nd	2d,2nt,2nd
4.7	0.1111	0.1134	0.0115	0.0114	0.0202	0.0287	3nd,1nt	5d,1t

Table 2: Comparison of Results: Near-Repeated Knots vs. Multiple Knots

We first describe the layout of the Table 2, which gives a comparison of the results of the simple knot and multiple knot algorithms for fourteen datasets. The results are for the surface fits obtained by starting from the initial guess obtained by the greedy algorithm [FH93], with $r = 0.3$, and closeness tolerance, ctol=0.1. The 3.n datasets were fit using twelve knot locations, while the 4.n datasets were fit using twenty knot locations. The columns of the table contain, in pairs, the values of r, the rms errors for the data points, the rms errors on a 21x21 grid, and information about the near-repeated or multiple knots obtained. The subscripts s and m denote the simple knot and multiple knot algorithms, respectively. The terms 2d and 1t, for example, refer to 2 double knots, and 1 triple knot. Likewise, 1nd refers to 1 near-double knot. In some cases two double knots may have been obtained, with another simple knot nearby one of the double knots - such a case might be denoted by 2d, 1nt.

For a given dataset, the values of r obtained are mostly comparable, with larger values generally being obtained by the multiple knot algorithm. In the instances where the value of r is not larger, the values are essentially the same, the exception being dataset 3.3. The cases showing the most difficulty are the cases 3.2 and 4.2 (the cliff function), which has a

6

tendency toward small values of the parameter r. The effects of this tendency are discussed in a later paragraph.

The rms errors are mostly comparable, with the errors obtained by the multiple knot algorithm generally smaller, with some ties, and one instance where the errors are bigger. This occurs for dataset 4.5, but the errors for both approximations are quite small for this case.

The rms errors on the grid ($grms$) generally follow the same pattern, with one major exception. On the dataset 3.2, the errors for the grid are quite large. Closer inspection of this particular case reveals there is one grid point (near the triple, almost quadruple, knot) where the surface is badly ill-behaved. Coefficients of the first derivative terms are on the order of 5 to 20, while the coefficients of the two multiquadric basis functions are reasonably large, on the order of 10^3. However, the value of r is very small in this case, about 1.5e-4, thus the derivatives of the basis functions very rapidly approach the value one in one of the coordinate directions (the value is about 0.99 at a distance of 0.001 from the knot). Hence, very rapid changes in the value of the function occur. While otherwise similar situations occur in other cases, the key difference here is the small value of r that occurs.

In order to discover whether the initial guess was contributing to the problem, or whether the tendency toward a small r value and multiple knots was driven by the data, we ran a number initial guesses for the datas t 3.2. The initial conditions were obtained from the greedy algorithm with various values of r and closeness tolerance (ctol). The results of the computations are summarized in Table 3. The table gives the parameter ctol, the initial value of r, the final value of r, the rms errors at the data points and on the grid, and the number, multiplicity, and approximate location of the multiple knots. From this we see that while there is a tendency toward multiple knots, no particular locations are tended toward, although it seems natural that repeated knots invariably occur near the diagonal. The fact that the surface is a function of one variable (that is, y-x) with rapid changes occurring near the diagonal may account for this circumstance. The fact that the data is not regular may account for a large number of comparable local minima. One case is of particular note: The case in the second line involves three triple and one double knot, however two of the triple knots are close together, yielding a near-repeated knot of multiplicity six. This could be expected to lead to poor behavior of the surface. Closer inspection revealed that, even though the coefficients are rather large (order 10^7), the surface is well behaved and yielded one of the better approximations among this group. This good behavior is undoubtedly enhanced by the fact that the r value is large for this surface. In the three cases where the r value is smaller than 10^{-4} the resulting surface is poorly behaved near a multiple or near-multiple knot, this being reflected by the larger $grms_o$ values shown.

We ran a number of different initial guesses for case 3.1 to determine both the robustness of the optimization routine and to confirm the tendency of the method to converge on multiple knots from a variety of initial guesses. Nine different initial guesses were made, six resulting from the greedy algorithm with different closeness tolerances and r values, and three with random initial knot locations. As is seen in Table 4, the results for the various initial guesses are strikingly similar: except for two cases the r values are all close to 0.16, all but one result in a triple or near-triple knot near the dip at about (.45,.78), and all but one have comparable accuracies for rms_o and $grms_o$. The one odd case had the starting value

7

of 0.01 for r. A wide-ranging difference is that different double and near-double knots may occur for the various runs. Unlike dataset 3.2, this case appears to be quite stable.

ctol	r	r_o	rms_o	$grms_o$	multiple knots
0.1	0.3	0.0002	0.0073	0.2496	t@(.09,.14), 3d@(.38,.38, (.60,.60), (.89,.88))
0.25	0.1	0.0239	0.0060	0.0085	3t@(.31,.36), (.76,.79), (.77,.78), 1d@(.12,.13)
0.1,	0.1	0.0247	0.0071	0.0111	2d@(.38,.40), (.67,.66)
0.2	0.1	0.0247	0.0071	0.0113	3d@(.14,.14),(.44,.44), (.68,.67)
0.25	0.01	0.0739	0.0054	0.0095	4d@(.13,.11),(.37,.39), (.69,.65), (.92,.91)
0.1	0.01	5e-5	0.0071	0.0259	d@(.69,.69), 2nd@(.14,.12), (.33,.40)
0.2	0.01	0.0001	0.0071	0.0114	d@(.44,.44)
0.0	0.01	5e-5	0.0071	0.0260	d@(.69,.69), 2nd@(.14,.11), (.33,.40)

Table 3: Results with Different Initial Guesses for Case 3.2

ctol	r	sk	r_o	rms_o	$grms_o$	multiple knots
0.0	0.3	g	0.1598	0.0067	0.0113	t@(.43,.76), 2nd@(.86,.23), (.83,.42)
0.1	0.3	g	0.1588	0.0059	0.0107	t@(.43,.75), d@(.78,.43), d is nt
0.2	0.3	g	0.1712	0.0063	0.0107	t@(.44,.74), d@(.15,.26)
0.25	0.3	g	0.2013	0.0075	0.0107	t@(.43,.79), d@(.20,.33)
0.1	0.1	g	0.1450	0.0066	0.0111	t@(.43,.77)
0.1	0.01	g	0.0737	0.0118	0.0157	d@(.72,.36)
-	0.3	r	0.1454	0.0066	0.0112	t@(.43,.77)
-	0.3	r	0.1566	0.0061	0.0077	t@(.42,.75)
-	0.3	r	0.1600	0.0067	0.0113	t@(.43,.76), 2nd@(.83,.43), (.86,.23)
-	0.3	r	0.1527	0.0067	0.0111	nt@(.44,.75)

Table 4: Results with Different Initial Guesses for Case 3.1

We also ran some different initial conditions on dataset 3.7. The results in this case seem to indicate complications somewhere between the datasets 3.1 and 3.2. Dataset 3.7 has a tendency toward many multiple knots, perhaps because it has a more complex behavior of the surface than any of the other datasets.

The occurrence of near-multiple knots, as we noted previously, must have a unfavorable effect on the condition number of the coefficient matrix, and in order to investigate this we computed the condition number of the coefficient matrices for the fourteen cases of Table 2. A plot of the of the minimum separation distance divided by the r value vs. the condition number of the coefficient matrix is shown in Figure 1. There are 15 points for each of the simple knot and multiple knot algorithms. The first fourteen points correspond to the data in Table 2, in the order given, while the fifteenth is for the thinned glacier dataset, GL, using 25 knots. For the latter data the underlying function is unknown. The simple knot algorithm found 9 near-double knots. The multiple knot algorithm found four double knots and three triple knots.

The points in Figure 1 for the simple knot algorithm have been labeled with their number. Because of the clustering of many of the points for the multiple knot algorithm, only those with condition number great than 10^5 have been labeled.

What can be observed is that the condition numbers for the multiple knot algorithm are generally one to two orders of magnitude smaller than those for the simple knot algorithm. There are exceptions to this, most notably the datasets 3.1, 3.2, 3.7, and 4.5, where the behavior is reversed, and 3.6 for which the r value is relatively large in both cases, contributing to the size of the condition number.

Finally, for one of the parent surfaces, we include a plot of the underlying surface being approximated, along with the surfaces obtained from the simple knot algorithm and the multiple knot algorithm. The dataset is 3.7, the surface shown in Figure 2a being sampled at 100 points. Figures 2b and 2c, respectively, show the surface reconstructed using the simple knot and multiple knot algorithms with twelve knot points. In this case it is clear that the multiple knot algorithm has achieved a better fit.

4   Conclusion and Ideas for Further Work

We have formulated an algorithm to allow coalescence of near-repeated knots into multiple knots, bringing into the approximation the appropriate derivatives of the basis function in place of the basis functions for the nearby knots. As a general rule, this results in both better approximations, and more stable computations, although individual examples do not conform to this ideal. Our computations convince us that the occurrence of multiple knots is a natural phenomenon, and that algorithms for the problem need to account for the possibility.

The tendency toward repeated knots leads to one possible idea for further exploration. This would be to begin initially with some (or all) knots being double knots to take advantage of the apparently greater fitting power of the multiquadric plus its directional derivative. We have not yet had the opportunity to pursue this idea. While the advantage of starting with multiple knots seems clear, the disadvantage is that coalescence of these knots skips odd-multiplicity knots, especially triple knots, which occur regularly in our computations.

We have observed the tendency toward repeated knots with the LEASTSQ algorithm and another (FMINS - see [WO85]) in the previous paper and feel the repeated knots are not occurring as an artifact of the optimization process. Nonetheless, an algorithm that took

advantage of the particular problem being solved could be more efficient and possibly avoid some of the local minima being found by the general minimization routines.

References

[DU76] J. Duchon, Splines minimizing rotation- invariant seminorms in Sobolev spaces, pp. 85-100 in **Mult' .ariate Approximation Theory**, W. Schempp K. Zeller (eds), Birkhäuser, 1979.

[FH93] R. Franke, H. Hagen, and G. M. Nielson, Least squares surface approximation to scattered data using multiquadric functions, to appear in **Adv. in Comput. Math.**

[FN91] R. Franke and G. M. Nielson, Scattered data interpolation and applications: A tutorial and survey, pp. 131-160 in **Geometric Modelling: Methods and Their Applications**, H. Hagen and D. Roller (eds), Springer- Verlag, 1991.

[FR82] R. Franke, Scattered data interpolation: Tests of some methods, **Math. Comp. 38** (1982) 181-200.

[HD72] R. L. Harder and R. N. Desmarais, Interpolation using surface splines, **J. Aircraft 9** (1972) 189-191.

[HA71] R. L. Hardy, Multiquadric equations of topography and other irregular surfaces, **J. Geophys. Res. 76** (1971) 1905-1915.

[HA90] R. L. Hardy, Theory and applications of the multiquadric-biharmonic method, **Comput. Math. Applics. 19** (1990) 163-208.

[MI86] C. A. Micchelli, Interpolation of scattered data: Distance matrices and conditionally positive definite functions, **Constr. Approx. 2** (1986) 11-22.

[MF92] J. McMahon and R. Franke, Knot selection for least squares thin plate splines, **SIAM J. Sci. Stat. Comput. 13** (1992) 484-498.

[NI78] G. M. Nielson, A first-order blending method for triangles based upon cubic interpolation, **Intern. J. Numer. Meth. Engr. 15** (1978) 308-318.

[NW91] F. J. Narcowich and J. W. Ward, Norms of inverses and condition numbers for matrices associated with scattered data, **J. Approx. Theory 64** (1991) 69-94.

[WO85] D. J. Woods, Dept. Math. Sciences, Rice Univ., Report 85-5, 1985.

Figure Captions

Figure 1: Minimum separation distance relative to r value vs. condition number for thirty problems. The o's denote simple knot cases, numbered from 1-15, the first 14 being as ordered in Table 2. Number 15 is the thinned glacier data, GL, with 25 knots. The x's denote the multiple knot cases - only those with condition number greater than 10^5 are labeled due to space considerations.

Figure 2: a) The parent surface from which the data was obtained. b) The surface obtained with 12 knots using the simple knot algorithm. c) The surface obtained with 12 knots using the multiple knot algorithm.
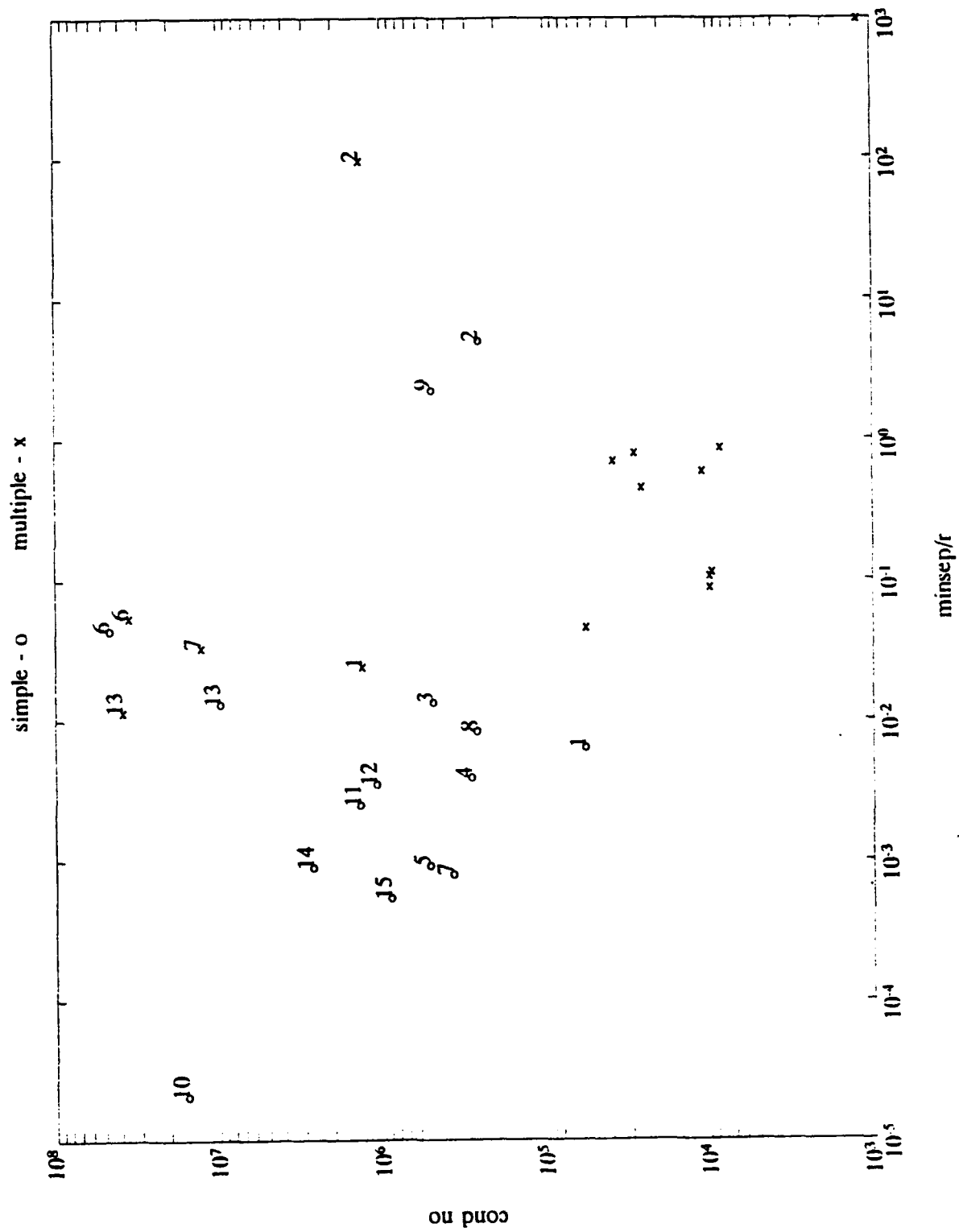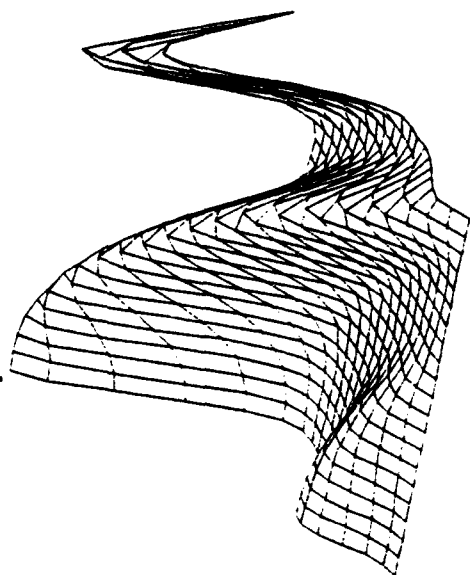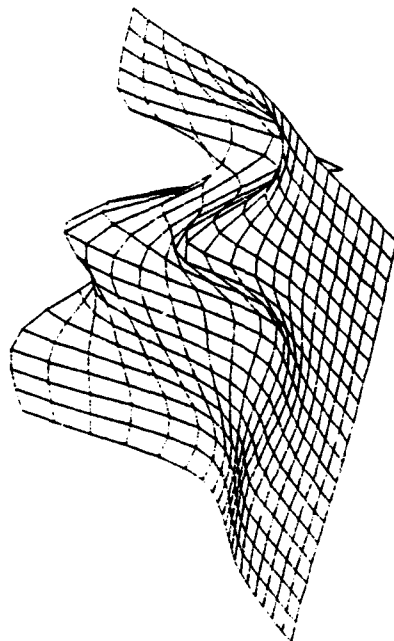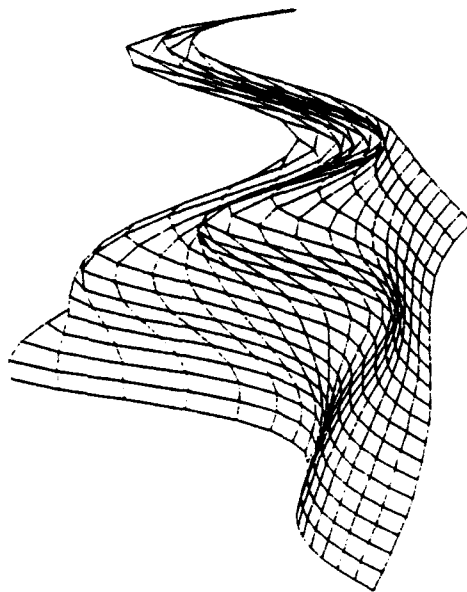
Figure 1

parent surface

a

simple knots

b

multiple knots

c

Figure 2

INITIAL DISTRIBUTION LIST

LIBRARY   (2)
NAVAL POSTGRADUATE SCHOOL
MONTEREY, CA 93943

DEAN OF RESEARCH   (2)
CODE 08
NAVAL POSTGRADUATE SCHOOL
MONTEREY, CA 93943

CHIEF OF NAVAL RESEARCH   (2)
LIBRARY SERVICES, CODE 784
BALLSTON TOWER #1
800 QUINCY ST.
ARLINGTON, VA 22217

DIRECTOR   (2)
DEFENSE TECH. INFORMATION
 CENTER, CAMERON STATION
ALEXANDRIA, VA 22314

DEPT. OF MATHEMATICS
NAVAL POSTGRADUATE SCHOOL
MONTEREY, CA 93943

PROFESSOR RICHARD FRANKE   (10)
CHAIRMAN, DEPT OF MATHEMATICS
NAVAL POSTGRADUATE SCHOOL
MONTEREY, CA 93943

PROFESSOR G. M. NIELSON   (5)
DEPT. OF COMPUTER SCIENCE
ARIZONA STATE UNIVERSITY
TEMPE, AZ 85287

PROFESSOR TOM FOLEY
DEPARTMENT OF COMPUTER SCIENCE
ARIZONA STATE UNIVERSITY
TEMPE, AZ 85327

DR. ROLLAND L. HARDY
INTERNATIONAL INSTITUTES OF
  SCIENCE AND TECHNOLOGY
484B WASHINGTON ST. SUITE 251
MONTEREY, CA 93940

DR. LARRY ROSENBLUM
OFFICE OF NAVAL RESEARCH
  EUROPEAN OFFICE
PSC 802 BOX 39
FPO AE 09499-0700

PROFESSOR DR. HANS HAGEN   (5)
FB INFORMATIK
UNIVERSITÄT KAISERSLAUTERN
6763 KAISERSLAUTERN
GERMANY

PROFESSOR DR. WILLI FREEDEN
FB MATHEMATIK
UNIVERSITÄT KAISERSLAUTERN
67653 KAISERSLAUTERN
GERMANY

DR. RICHARD LAU
OFFICE OF NAVAL RESEARCH
800 QUINCY ST.
ARLINGTON, VA 22217

DR. EDWARD BARKER
MS. NANCY BAKER
NAVAL RESEARCH LABORATORY/
  MONTEREY
MONTEREY, CA 93943

PROFESSOR PETER ALFELD
DEPARTMENT OF MATHEMATICS
UNIVERSITY OF UTAH
SALT LAKE CITY, UT 84112

PROFESSOR R.E. BARNHILL
DEPT. OF COMPUTER SCIENCE
ARIZONA STATE UNIVERSITY
TEMPE, AZ 85287

DR. RALPH CARLSON
L 316
LAWRENCE LIVERMORE NATIONAL LAB
LIVERMORE, CA 94550

DR. EDWARD J. KANSA
L 200
LAWRENCE LIVERMORE NATIONAL LAB
LIVERMORE, CA 94550

PROF. DR. GUIDO BRUNNETT
FB INFORMATIK
UNIVERSITÄT KAISERSLAUTERN
67653 KAISERSLAUTERN
GERMANY